Induced Variational Method from Supersymmetric Quantum Mechanics and the Screened Coulomb Potential [1]

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Abstract
The formalism of Supersymmetric Quantum Mechanics supplies a trial wave function to be used in the Variational Method. The screened Coulomb potential is analysed within this approach. Numerical and exact results for energy eigenvalues are compared.

I. Introduction

The screened Coulomb potential has been used in several branches of Physics, for instance, in nuclear physics (as the name of Yukawa potential), in plasma and in the study of electrolytic solution properties (Debye-Huckel potential). The Schrödinger equation for this potential is not exactly solvable and exact numerical, [1], [2] and approximative, [3]-[5] methods have been applied to obtain the energy eigenvalues, including variational calculations, [6]-[8].

More recently, a new methodology based within the variational method associated to supersymmetric quantum mechanics formalism has been introduced, [9]-[11]. References [9] and [10] introduce a scheme based in the hierarchy of Hamiltonians; it permits the evaluation of excited states for one-dimensional systems. In reference [11] an *ansatz* for the superpotential which is related to the trial wave function is proposed. The new approach showed to be useful to get answers when applied to atomic systems, [11]-[12].

In this letter, the variational energy eigenvalues for the static screened Coulomb potential in three dimensions are determined using the variational method using a trial wave function induced by Supersymmetric Quantum Mechanics, SQM.

In the approach followed here the first step taken is to look for an effective potential similar to the original screened Coulomb potential. Inspired by SQM, an *ansatz* is

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made to the superpotential which determines the variational (trial) wavefunction through the algebraic approach of SQM.

Our system is three dimensional and in this case it is possible to determine the variational eigenfunctions for each value of angular momentum l. The first eigenfunction, obtained from direct factorization of the effective Hamiltonian, corresponds to the minimum energy for each l.

This new methodology has been successfully applied to other atomic systems such as the Hulthén, [11], and the Morse, [12], potentials. Here it is applied to the screened Coulomb potential.

In what follows, we briefly introduce, for completeness, the SQM scheme, then introduce the variational method and show our results.

II. Supersymmetric Quantum Mechanics

In SQM, [10]-[11], for $N = 2$ we have two nilpotent operators, Q and Q^+, that satisfying the algebra

$$\{Q, Q^+\} = H_{SS} \quad ; Q^2 = {Q^+}^2 = 0, \tag{1}$$

where H_{SS} is the supersymmetric Hamiltonian. This algebra can be realized as

$$Q = \begin{pmatrix} 0 & 0 \\ A^- & 0 \end{pmatrix}, \quad Q^+ = \begin{pmatrix} 0 & A^+ \\ 0 & 0 \end{pmatrix} \tag{2}$$

where $A^\pm$ are bosonic operators. With this realization the supersymmetric Hamiltonian H_{SS} is then given by

$$H_{SS} = \begin{pmatrix} A^+A^- & 0 \\ 0 & A^-A^+ \end{pmatrix} = \begin{pmatrix} H^+ & 0 \\ 0 & H^- \end{pmatrix}. \tag{3}$$

where $H^\pm$ are called supersymmetric partner Hamiltonians and share the same spectra, apart from the nondegenerate ground state. Using the super-algebra, a given Hamiltonian can be factorized in terms of the bosonic operators. In $\hbar = c = 1$ units, it is given by

$$H_1 = -\frac{1}{2}\frac{d^2}{dr^2} + V_1(r) = A_1^+ A_1^- + E_0^{(1)} \tag{4}$$

where $E_0^{(1)}$ is the lowest eigenvalue and the function $V_1(r)$ includes the barrier potential term. The bosonic operators are defined by

$$A_1^\pm = \frac{1}{\sqrt{2}}\left(\mp\frac{d}{dr} + W_1(r)\right) \tag{5}$$

where the superpotential $W_1(r)$ satisfies the Riccati equation

$$W_1^2 - W_1' = 2V_1(r) - 2E_0^{(1)} \tag{6}$$

which is a consequence of the factorization of the Hamiltonian H_1.

The eigenfunction for the lowest state is related to the superpotential W_1 by

$$\Psi_0^{(1)}(r) = Nexp(-\int_0^r W_1(\bar{r})d\bar{r}). \tag{7}$$

Now it is possible to construct the supersymmetric partner Hamiltonian

$$H_2 = A_1^- A_1^+ + E_0^{(1)} = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{1}{2}(W_1^2 + W_1') + E_0^{(1)}. \tag{8}$$

If one factorizes H_2 in terms of a new pair of bosonic operators, $A_2^{\pm}$ one gets,

$$H_2 = A_2^+ A_2^- + E_0^{(2)} = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{1}{2}(W_2^2 - W_2') + E_0^{(2)} \tag{9}$$

where $E_0^{(2)}$ is the lowest eigenvalue of H_2 and W_2 satisfy the Riccati equation,

$$W_2^2 - W_2' = 2V_2(r) - 2E_0^{(2)}. \tag{10}$$

Thus a whole hierarchy of Hamiltonians can be constructed, with simple relations connecting the eigenvalues and eigenfunctions of the n-members, [13], [15].

Thus, the formalism of SQM allows us to evaluate the ground state eigenfunction from the knowledge of the superpotential $W(r)$, satisfying the Riccati equation, eq.(6). However, since the potential is not exactly solvable, the purpose is to propose an *ansatz* for the superpotential and, based in the superalgebra information, we evaluate a trial wavefunction that minimizes the expectation value of the energy. The energy eigenvalues pursued are evaluated by minimizing the energy expectation value with respect to a free parameter introduced by the *ansatz*.

III. Trial wavefunction for the variational calculation

The screened Coulomb potential is given, in atomic units, by

$$V_{SC} = -\frac{e^{-\delta r}}{r} \tag{11}$$

where δ is the screened length. The associated radial Schrödinger equation includes the potential barrier term and it is given by

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} - \frac{e^{-\delta r}}{r} + \frac{l(l+1)}{2r^2}\right)\Psi = E\Psi \tag{12}$$

where the unit length is $\hbar^2/me^2$ and the energy unit is $\epsilon_0 = -me^4/\hbar^2$.

In order to determine an effective potential similar to the potential in the Hamiltonian (12), that is the screened Coulomb potential plus the potential barrier term, the following *ansatz* to the superpotential is suggested

$$W(r) = -(l+1)\frac{\delta e^{-\delta r}}{1-e^{-\delta r}} + \frac{1}{(l+1)} - \frac{\delta}{2}. \tag{13}$$

Substituting it into (7), one gets

$$\Psi_0(r) = (1 - e^{-\delta r})^{l+1} e^{-(\frac{1}{(l+1)} - \frac{\delta}{2})r}. \tag{14}$$

Assuming that the radial trial wave function is given by (14), replacing δ by the variational parameter μ, i.e.,

$$\Psi_\mu(r) = (1 - e^{-\mu r})^{l+1} e^{-(\frac{1}{(l+1)} - \frac{\mu}{2})r}, \tag{15}$$

the variational energy is given by

$$E_\mu = \frac{\int_0^\infty \Psi_\mu(r)[-\frac{1}{2}\frac{d^2}{dr^2} - \frac{e^{-\delta r}}{r} + \frac{l(l+1)}{2r^2}]\Psi_\mu(r)dr}{\int_0^\infty \Psi_\mu(r)^2 dr}. \tag{16}$$

Thus, minimizing this energy with respect to the variational parameter μ one obtains the best estimate for the energy of the screened Coulomb potential.

As our potential is not exactly solvable, the superpotential given by eq.(13) does not satisfy the Riccati equation (6) but it does satisfy it for an effective potential instead, V_{eff}

$$V_{eff}(r) = \frac{\bar{W}_1^2 - \bar{W}_1'}{2} + E(\bar{\mu}) \tag{17}$$

where $\bar{W}_1 = W_1(\delta = \bar{\mu})$ is given by eq.(13) and $\bar{\mu}$ is the parameter that minimises the energy expectation value, (16). It is given by

$$V_{eff}(r) = -\frac{\delta e^{-\delta r}}{1 - e^{-\delta r}} + \frac{l(l+1)}{2}\frac{\delta^2 e^{-2\delta r}}{(1 - e^{-\delta r})^2} + \frac{1}{2}(\frac{1}{l+1} - \frac{\delta}{2})^2 + E(\delta), \tag{18}$$

where $\delta = \bar{\mu}$ that minimises energy expectation value. One observes that for small values of δ the first term is similar to the potential (11) and the last is approximately the potential barrier term. This observation allows us to conclude that the superpotential (13) can be used to analyse the three dimensional screened Coulomb potential variationally through the trial wavefunction (14).

IV. Results

For $l = 0$ the effective potential (18) becomes identical to the Hulthén potential. Thus, the results presented in Table 1 coincide with those of ref.[7], where the Hulthén potential eigenfunctions are directly used in the variational calculation. The deviation on the fifth decimal algarism can be attributed to the accuracy of the numerical calculation.

State 1s			
Screening δ	SQM Variational	Variational (Ref. 7)	Exact Numerical
0.001	-0.49902	-0.49900	-
0.002	0.49802	-0.49800	-0.4980
0.005	-0.49504	-0.49502	-0.4950
0.010	-0.49009	-0.49007	-0.4901
0.02	-0.48031	-0.48030	-0.4803
0.025	-047548	-0.47546	-0.4755
0.03	-0.47068	-0.47066	-
0.04	-0.46119	-0.46117	-
0.05	-0.45180	-0.45182	-0.4518
0.06	-0.44259	-0.44260	-
0.07	-0.43351	-0.43352	-
0.08	-0.42456	-0.42457	-
0.09	-0.41574	-0.41575	-
0.10	-0.40705	-0.40706	-0.4071
0.20	-0.32681	-0.32681	-0.3268
0.25	-0.29092	-0.29092	-0.2909
0.30	-0.25764	-0.25763	-
0.40	-0.19842	-0.19836	-
0.50	-0.14806	-0.14808	-0.1481
0.60	-0106077	-0.10608	-
0.70	-0.07175	-0.07174	-
0.80	-0.04459	-0.04459	-
0.90	-0.02420	-0.02418	-
1.00	-0.01026	-0.01016	-0.01029
1.05	-0.00568	-0.00544	-

Table 1. Energy eigenvalues as function of the screening parameters δ for $1s$ state ($l = 0$), in rydberg units of energy. Comparison is make with variational and exact numerical results from [1] and [7].

The results become more interesting for $l \neq 0$. In this case the effective potential differs from the Hulthén potential. Table 2 shows the results for $2p$ ($l = 1$), $3d$ ($l = 2$) and $4f$ ($l = 3$) energy levels. Also given in this table are the correponding numerical results [1].

	2p		3d		4f	
δ	Variational	Numerical	Variational	Numerical	Variational	Numerical
0.001	-0.2480	-0.2480	-0.10910	-0.10910	-0.06051	-0.06052
0.005	-	-	-	-	-0.52930	-0.05294
0.010	-0.2305	-0.2305	-0.09212	-0.09212	-0.04419	-0.04420
0.020	-0.2119	-0.2119	-0.07503	-0.07503	-0.02897	-0.02898
0.025	-0.2030	-0.2030	-0.06714	-0.06715	-	-
0.050	-0.1615	-0.1615	-0.03374	-0.03383	-	-
0.100	-0.09289	-0.09307	-	-	-	-

Table 2. Energy eigenvalues as function of the screening parameters δ for $2p$ ($l = 1$), $3d$ ($l = 2$) and $4f$ ($l = 3$) states, in rydberg units of energy. Variational values obtained by the trial function (15) are compared with exact numerical results obtained from reference [1], (see also [6]).

V. Conclusions

We have proposed trial wavefunctions to be used in the variational calculation in order to determine the energy eigenvalues of the screened Coulomb potential. These functions were induced from supersymmetric quantum mechanics formalism. The approach consists of making an *ansatz* in the superpotential which satifies the Riccati equation by an effective potential. The trial wavefunctions were then determined from this superpotential through the superalgebra.

For $l = 0$ the effective potential obtained is identical to the Hulthén potential. However for $l \neq 0$ the potential has a new structure. The trial wavefunctions suggested for this case are different from those proposed in references [6]-[8]. Within our framework the energy eigenvalue for each value of l is obtained using the same function (14).

In terms of the hierarchy of Hamiltonians, we obtained the first member for each value of l. Other members can be determined from the usual approach in supersymmetric quantum mechanics, [15].

One observes that the results obtained are in very good agreement to those found in the literature. The results are better for small values of the parameter δ. This observation is justified by the fact that for small values of δ the effective potential is more similar to the original potential than for higher values of δ.

We stress that even though the problem has been attacked by different methods our new methodology is very simple to supply accurate results. We believe that other applications to atomic physics problems can be made by this new method.

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